



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:57 PM UTC

PDB ID : 4UBD / pdb_00004ubd
Title : Crystal structure of a neutralizing human monoclonal antibody with 1968 H3 HA
Authors : Shore, D.A.; Yang, H.; Cho, M.; Donis, R.O.; Stevens, J.
Deposited on : 2014-08-12
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

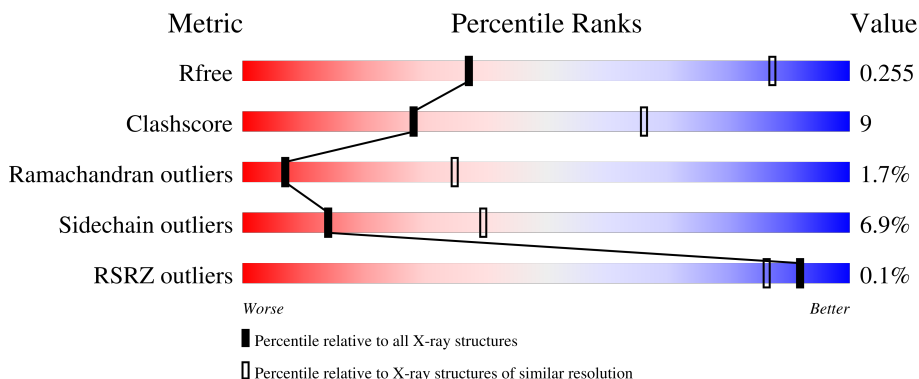
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


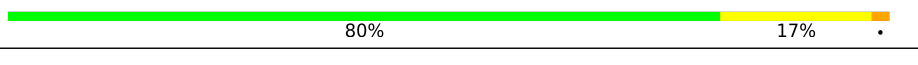
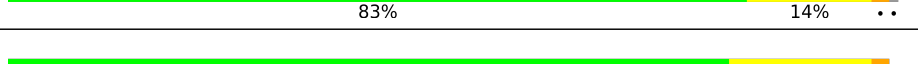
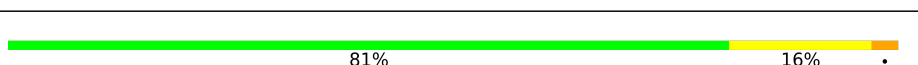

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






















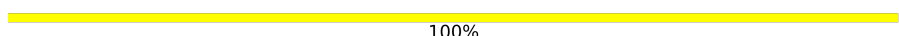


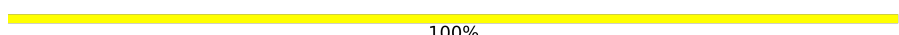


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	 82% 14% ..
1	E	321	 80% 17% .
1	I	321	 83% 14% ..
1	M	321	 81% 16% .
1	Q	321	 81% 16% .


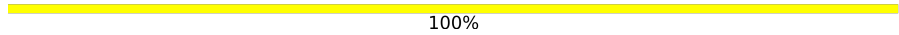
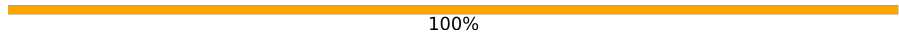
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Mol	Chain	Length	Quality of chain
1	U	321	 82% 16%
2	B	175	 76% 14% 5% 6%
2	F	175	 70% 19% 7%
2	J	175	 75% 16% 6%
2	N	175	 74% 16% 7%
2	R	175	 73% 17% 5% 5%
2	V	175	 77% 17% 6%
3	C	226	 72% 18% 6%
3	G	226	 72% 19%
3	K	226	 73% 19%
3	O	226	 72% 19%
3	S	226	 72% 19% 5%
3	Y	226	 73% 19% 5%
4	D	215	 80% 16%
4	H	215	 78% 18%
4	L	215	 82% 14%
4	P	215	 81% 15%
4	T	215	 79% 17%
4	X	215	 81% 17%
5	W	4	 100%
5	b	4	 25% 75%
5	c	4	 75% 25%
5	d	4	 100%
5	e	4	 75% 25%
5	g	4	 25% 75%

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Mol	Chain	Length	Quality of chain
6	Z	2	 50% 50%
6	a	2	 100%
6	f	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	W	4	X	-	-	-
5	MAN	b	4	X	-	-	-
5	MAN	c	4	X	-	-	-
5	MAN	d	4	X	-	-	-
5	MAN	e	4	X	-	-	-
5	MAN	g	4	X	-	-	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 43086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2470	1546	434	477	13	0	0	0
1	U	320	2470	1546	434	477	13	0	0	0
1	I	317	2445	1531	429	472	13	0	0	0
1	M	320	2470	1546	434	477	13	0	0	0
1	Q	320	2470	1546	434	477	13	0	0	0
1	E	320	2470	1546	434	477	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	GLN	-	expression tag	UNP Q91MA7
U	329	GLN	-	expression tag	UNP Q91MA7
I	329	GLN	-	expression tag	UNP Q91MA7
M	329	GLN	-	expression tag	UNP Q91MA7
Q	329	GLN	-	expression tag	UNP Q91MA7
E	329	GLN	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	V	164	1346	831	238	271	6	0	0	0
2	F	163	1338	825	237	270	6	0	0	0
2	B	165	1357	840	239	272	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	164	Total	C	N	O	S	0	0	0
			1349	834	238	271	6			
2	N	163	Total	C	N	O	S	0	0	0
			1338	825	237	270	6			
2	R	166	Total	C	N	O	S	0	0	0
			1359	839	241	273	6			

- Molecule 3 is a protein called monoclonal antibody H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1637	1036	278	319	4			
3	Y	219	Total	C	N	O	S	0	0	0
			1637	1036	278	319	4			
3	G	219	Total	C	N	O	S	0	0	0
			1637	1036	278	319	4			
3	S	219	Total	C	N	O	S	0	0	0
			1637	1036	278	319	4			
3	O	219	Total	C	N	O	S	0	0	0
			1637	1036	278	319	4			
3	K	219	Total	C	N	O	S	0	0	0
			1637	1036	278	319	4			

- Molecule 4 is a protein called monoclonal antibody L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	213	Total	C	N	O	S	0	0	0
			1650	1029	290	327	4			
4	X	213	Total	C	N	O	S	0	0	0
			1650	1029	290	327	4			
4	H	213	Total	C	N	O	S	0	0	0
			1650	1029	290	327	4			
4	T	213	Total	C	N	O	S	0	0	0
			1650	1029	290	327	4			
4	P	213	Total	C	N	O	S	0	0	0
			1650	1029	290	327	4			
4	L	213	Total	C	N	O	S	0	0	0
			1650	1029	290	327	4			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	W	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	b	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	c	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	d	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	e	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	g	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	f	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

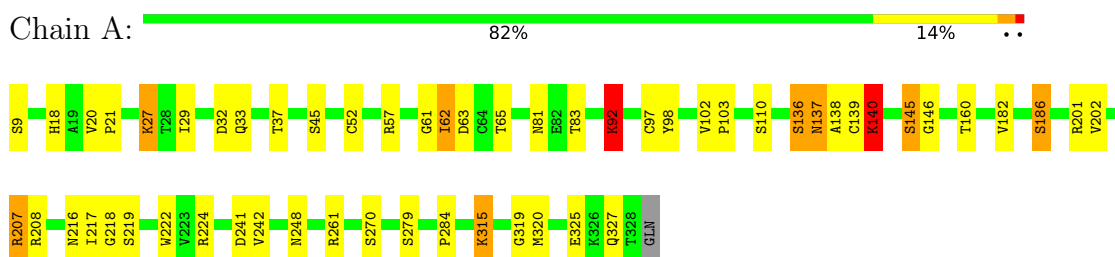


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	Total 14	8	1	5	0	0
7	U	1	Total 14	8	1	5	0	0
7	V	1	Total 14	8	1	5	0	0
7	I	1	Total 14	8	1	5	0	0
7	M	1	Total 14	8	1	5	0	0
7	Q	1	Total 14	8	1	5	0	0
7	F	1	Total 14	8	1	5	0	0

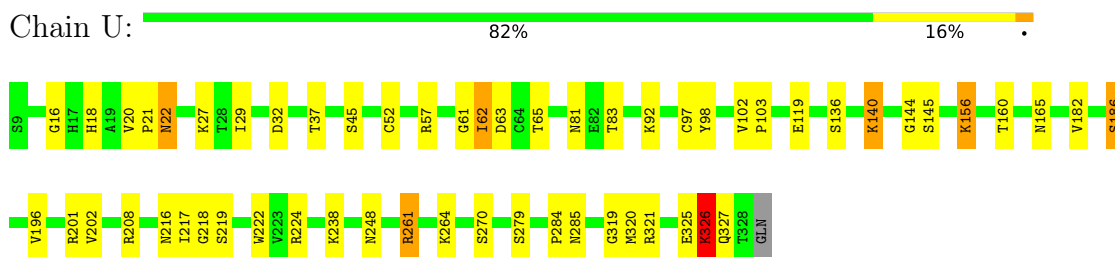
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

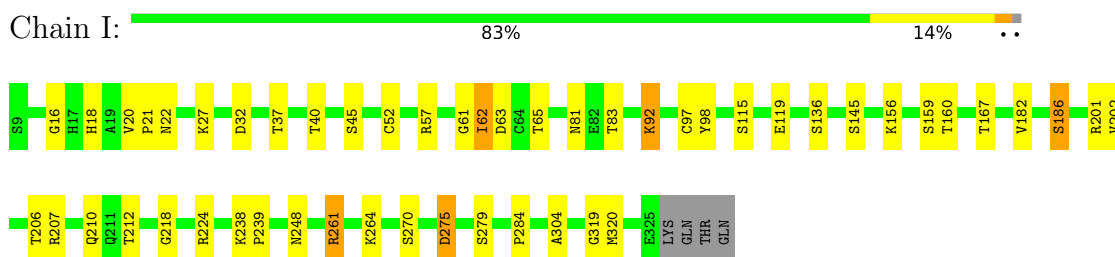
- Molecule 1: Hemagglutinin HA1 chain



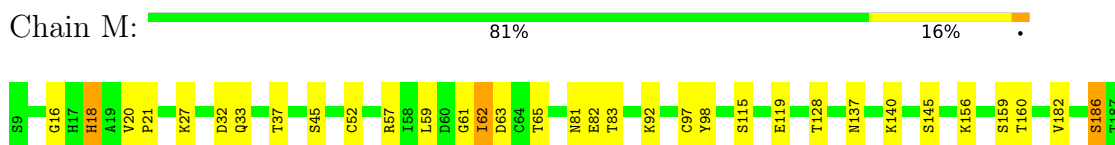
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

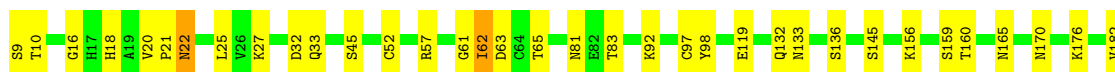
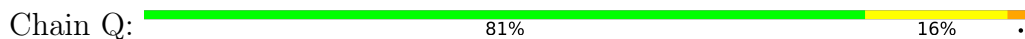


- Molecule 1: Hemagglutinin HA1 chain

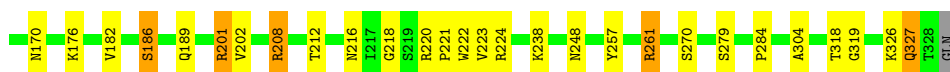
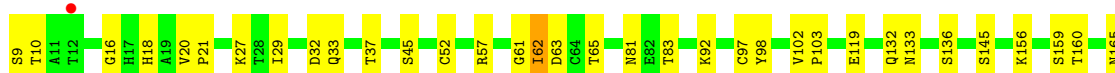




- Molecule 1: Hemagglutinin HA1 chain



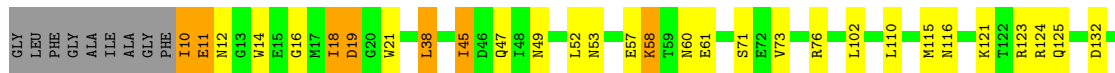
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain

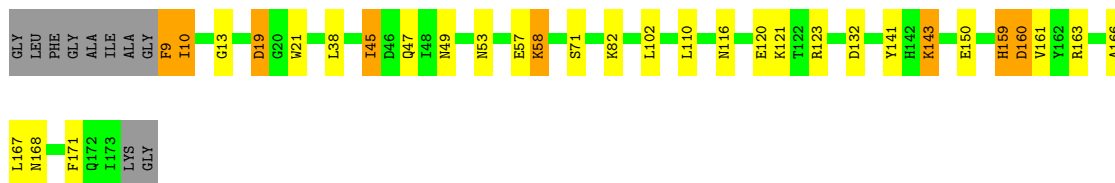


- Molecule 2: Hemagglutinin HA2 chain



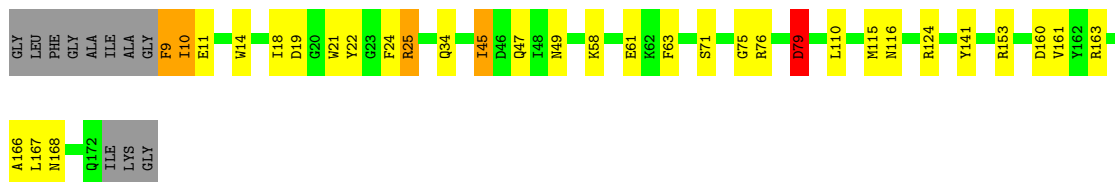
- Molecule 2: Hemagglutinin HA2 chain





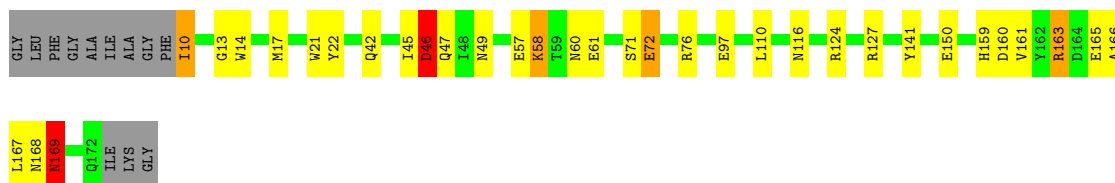
- Molecule 2: Hemagglutinin HA2 chain

Chain J: 75% 16% •• 6%



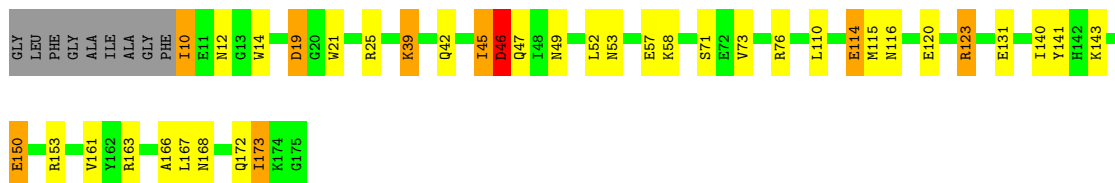
- Molecule 2: Hemagglutinin HA2 chain

Chain N: 74% 16% •• 7%



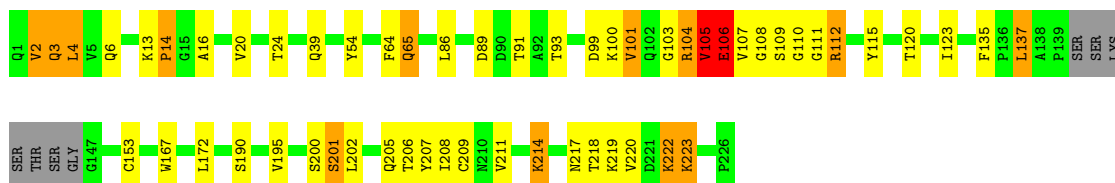
- Molecule 2: Hemagglutinin HA2 chain

Chain R: 73% 17% 5% • 5%



- Molecule 3: monoclonal antibody H chain

Chain C: 72% 18% 6% ••



- Molecule 3: monoclonal antibody H chain

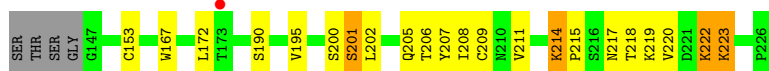
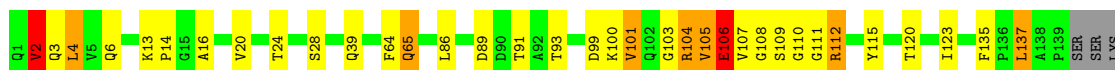
Chain Y: 73% 19% 5% ••



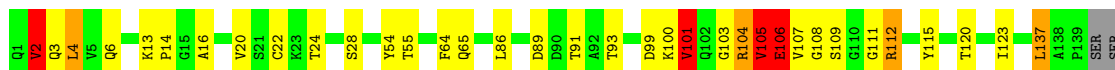
• Molecule 3: monoclonal antibody H chain



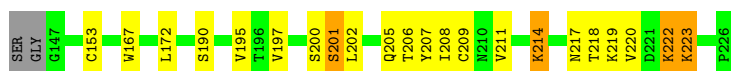
• Molecule 3: monoclonal antibody H chain




• Molecule 3: monoclonal antibody H chain

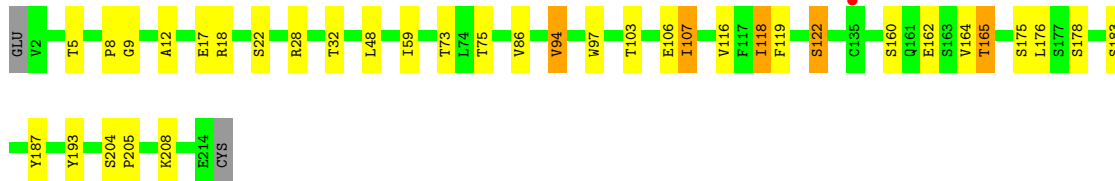


• Molecule 3: monoclonal antibody H chain



• Molecule 4: monoclonal antibody L chain

Chain L:  82% 14% ..



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  25% 75%

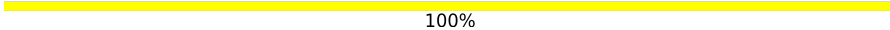


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  75% 25%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	128.70Å 128.70Å 428.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.50) 99.4 (50.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.258 0.216 , 0.255	Depositor DCC
R_{free} test set	4962 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.006 for -h,-k,l 0.410 for h,-h-k,-l 0.018 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	43086	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.82	0/2526	1.00	3/3442 (0.1%)
1	E	0.83	0/2526	0.97	1/3442 (0.0%)
1	I	0.85	1/2501 (0.0%)	0.98	0/3409
1	M	0.84	2/2526 (0.1%)	0.97	2/3442 (0.1%)
1	Q	0.83	0/2526	0.98	1/3442 (0.0%)
1	U	0.82	0/2526	0.98	1/3442 (0.0%)
2	B	0.99	1/1380 (0.1%)	1.09	3/1855 (0.2%)
2	F	0.96	1/1360 (0.1%)	1.12	6/1828 (0.3%)
2	J	0.94	1/1372 (0.1%)	1.11	5/1844 (0.3%)
2	N	0.95	2/1360 (0.1%)	1.17	8/1828 (0.4%)
2	R	0.99	2/1381 (0.1%)	1.18	10/1855 (0.5%)
2	V	0.98	3/1368 (0.2%)	1.09	3/1839 (0.2%)
3	C	0.83	0/1677	1.03	5/2289 (0.2%)
3	G	0.82	0/1677	1.02	4/2289 (0.2%)
3	K	0.74	0/1677	0.97	3/2289 (0.1%)
3	O	0.74	1/1677 (0.1%)	0.98	2/2289 (0.1%)
3	S	0.83	0/1677	1.02	4/2289 (0.2%)
3	Y	0.83	0/1677	1.03	5/2289 (0.2%)
4	D	0.82	0/1687	0.98	1/2292 (0.0%)
4	H	0.85	0/1687	0.98	2/2292 (0.1%)
4	L	0.68	0/1687	0.93	1/2292 (0.0%)
4	P	0.70	0/1687	0.93	1/2292 (0.0%)
4	T	0.86	2/1687 (0.1%)	0.99	2/2292 (0.1%)
4	X	0.83	0/1687	0.98	1/2292 (0.0%)
All	All	0.84	16/43536 (0.0%)	1.01	74/59154 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	G	0	1
3	K	0	1
3	O	0	1
3	S	0	1
3	Y	0	1
All	All	0	6

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	120	PRO	CA-C	6.07	1.55	1.51
2	B	19	ASP	CA-C	5.99	1.60	1.52
3	O	101	VAL	C-O	-5.96	1.17	1.24
1	I	275	ASP	CB-CG	5.84	1.66	1.52
2	V	10	ILE	CA-CB	5.73	1.70	1.54

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	46	ASP	N-CA-CB	9.93	125.51	110.22
2	N	46	ASP	N-CA-CB	9.55	125.23	110.14
1	U	156	LYS	CB-CA-C	-9.16	93.43	109.64
3	Y	223	LYS	N-CA-C	8.77	123.23	109.81
3	C	223	LYS	N-CA-C	8.69	122.92	110.14

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	106	GLU	Peptide
3	G	106	GLU	Peptide
3	O	106	GLU	Peptide
3	S	106	GLU	Peptide
3	Y	106	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2470	0	2419	59	0
1	E	2470	0	2422	48	0
1	I	2445	0	2393	31	1
1	M	2470	0	2421	40	1
1	Q	2470	0	2420	45	0
1	U	2470	0	2421	49	0
2	B	1357	0	1275	24	0
2	F	1338	0	1255	27	0
2	J	1349	0	1264	20	0
2	N	1338	0	1255	23	0
2	R	1359	0	1282	24	0
2	V	1346	0	1265	16	0
3	C	1637	0	1610	58	0
3	G	1637	0	1610	57	0
3	K	1637	0	1610	51	0
3	O	1637	0	1610	51	0
3	S	1637	0	1610	63	0
3	Y	1637	0	1610	56	0
4	D	1650	0	1602	21	0
4	H	1650	0	1602	27	1
4	L	1650	0	1602	24	0
4	P	1650	0	1602	23	0
4	T	1650	0	1602	26	1
4	X	1650	0	1602	17	0
5	W	50	0	43	0	0
5	b	50	0	43	2	0
5	c	50	0	43	1	0
5	d	50	0	43	0	0
5	e	50	0	43	2	0
5	g	50	0	43	2	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
6	f	28	0	25	7	0
7	A	14	0	13	0	0
7	F	14	0	13	0	0
7	I	14	0	13	2	0
7	M	14	0	13	0	0
7	Q	14	0	13	0	0
7	U	14	0	13	5	0
7	V	14	0	13	0	0
All	All	43086	0	41788	752	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 752 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:285:ASN:ND2	7:U:405:NAG:C1	1.71	1.51
1:U:156:LYS:HE2	1:U:196:VAL:CG2	1.66	1.25
1:A:140:LYS:HD2	1:A:140:LYS:N	1.33	1.22
1:U:156:LYS:CE	1:U:196:VAL:HG23	1.75	1.16
3:G:208:ILE:HA	3:G:223:LYS:HD3	1.21	1.11

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:275:ASP:OD1	4:T:188:GLU:OE2[1_445]	1.91	0.29
1:I:275:ASP:OD1	4:H:188:GLU:OE2[1_565]	1.92	0.28

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/321 (99%)	297 (93%)	18 (6%)	3 (1%)	14	47
1	E	318/321 (99%)	300 (94%)	15 (5%)	3 (1%)	14	47
1	I	315/321 (98%)	297 (94%)	16 (5%)	2 (1%)	21	54
1	M	318/321 (99%)	297 (93%)	18 (6%)	3 (1%)	14	47
1	Q	318/321 (99%)	300 (94%)	15 (5%)	3 (1%)	14	47
1	U	318/321 (99%)	296 (93%)	19 (6%)	3 (1%)	14	47
2	B	163/175 (93%)	150 (92%)	13 (8%)	0	100	100
2	F	161/175 (92%)	151 (94%)	10 (6%)	0	100	100
2	J	162/175 (93%)	149 (92%)	13 (8%)	0	100	100
2	N	161/175 (92%)	150 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	164/175 (94%)	151 (92%)	12 (7%)	1 (1%)	21	54
2	V	162/175 (93%)	149 (92%)	13 (8%)	0	100	100
3	C	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	1	15
3	G	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	1	15
3	K	215/226 (95%)	189 (88%)	17 (8%)	9 (4%)	2	19
3	O	215/226 (95%)	189 (88%)	16 (7%)	10 (5%)	2	17
3	S	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	1	15
3	Y	215/226 (95%)	189 (88%)	17 (8%)	9 (4%)	2	19
4	D	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	14	47
4	H	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	14	47
4	L	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	14	47
4	P	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	14	47
4	T	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	14	47
4	X	211/215 (98%)	202 (96%)	7 (3%)	2 (1%)	14	47
All	All	5434/5622 (97%)	5023 (92%)	320 (6%)	91 (2%)	7	35

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	327	GLN
3	C	104	ARG
3	C	105	VAL
3	C	109	SER
3	Y	104	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/283 (100%)	268 (95%)	14 (5%)	22	48
1	E	282/283 (100%)	269 (95%)	13 (5%)	24	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	279/283 (99%)	269 (96%)	10 (4%)	31	57
1	M	282/283 (100%)	269 (95%)	13 (5%)	24	50
1	Q	282/283 (100%)	266 (94%)	16 (6%)	18	45
1	U	282/283 (100%)	266 (94%)	16 (6%)	18	45
2	B	145/149 (97%)	133 (92%)	12 (8%)	10	34
2	F	143/149 (96%)	131 (92%)	12 (8%)	10	34
2	J	144/149 (97%)	134 (93%)	10 (7%)	14	39
2	N	143/149 (96%)	133 (93%)	10 (7%)	14	39
2	R	145/149 (97%)	132 (91%)	13 (9%)	9	32
2	V	144/149 (97%)	137 (95%)	7 (5%)	22	48
3	C	181/187 (97%)	167 (92%)	14 (8%)	12	37
3	G	181/187 (97%)	167 (92%)	14 (8%)	12	37
3	K	181/187 (97%)	167 (92%)	14 (8%)	12	37
3	O	181/187 (97%)	167 (92%)	14 (8%)	12	37
3	S	181/187 (97%)	168 (93%)	13 (7%)	13	38
3	Y	181/187 (97%)	167 (92%)	14 (8%)	12	37
4	D	184/186 (99%)	168 (91%)	16 (9%)	9	33
4	H	184/186 (99%)	167 (91%)	17 (9%)	8	32
4	L	184/186 (99%)	168 (91%)	16 (9%)	9	33
4	P	184/186 (99%)	167 (91%)	17 (9%)	8	32
4	T	184/186 (99%)	168 (91%)	16 (9%)	9	33
4	X	184/186 (99%)	167 (91%)	17 (9%)	8	32
All	All	4743/4830 (98%)	4415 (93%)	328 (7%)	14	39

5 of 328 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	118	ILE
4	P	75	THR
3	S	4	LEU
4	T	107	ILE
3	K	89	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	210	ASN
4	P	148	GLN
4	H	54	ASN
4	T	139	ASN
4	L	43	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

25 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Q	407	1	14,14,15	1.43	3 (21%)	17,19,21	3.39	9 (52%)
5	NAG	W	2	5	14,14,15	0.69	0	17,19,21	2.61	7 (41%)
6	NAG	a	1	1,6	14,14,15	1.02	1 (7%)	17,19,21	2.31	7 (41%)
7	NAG	F	201	-	14,14,15	0.99	0	17,19,21	2.24	5 (29%)
5	NAG	e	2	5	14,14,15	0.56	0	17,19,21	2.44	7 (41%)
7	NAG	U	405	-	14,14,15	1.34	2 (14%)	17,19,21	2.96	9 (52%)
5	NAG	b	1	1,5	14,14,15	0.73	0	17,19,21	1.77	4 (23%)
5	NAG	g	2	5	14,14,15	0.79	0	17,19,21	3.26	10 (58%)
5	NAG	d	1	1,5	14,14,15	0.54	0	17,19,21	2.18	4 (23%)
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	2.57	8 (47%)
6	NAG	f	1	1,6	14,14,15	1.15	1 (7%)	17,19,21	2.95	7 (41%)
7	NAG	A	409	1	14,14,15	1.06	1 (7%)	17,19,21	3.33	8 (47%)
6	NAG	f	2	6	14,14,15	0.86	0	17,19,21	1.79	5 (29%)
6	NAG	Z	1	1,6	14,14,15	0.91	1 (7%)	17,19,21	2.70	6 (35%)
7	NAG	M	405	1	14,14,15	1.09	1 (7%)	17,19,21	1.34	3 (17%)
5	NAG	c	1	1,5	14,14,15	0.80	0	17,19,21	3.90	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	W	1	1,5	14,14,15	0.70	0	17,19,21	1.67	4 (23%)
6	NAG	Z	2	6	14,14,15	0.76	0	17,19,21	1.73	3 (17%)
5	NAG	c	2	5	14,14,15	0.83	1 (7%)	17,19,21	3.80	10 (58%)
6	NAG	a	2	6	14,14,15	0.86	1 (7%)	17,19,21	2.24	7 (41%)
7	NAG	I	405	1	14,14,15	1.68	2 (14%)	17,19,21	3.24	11 (64%)
5	NAG	g	1	1,5	14,14,15	0.69	0	17,19,21	1.49	3 (17%)
7	NAG	V	201	2	14,14,15	1.05	1 (7%)	17,19,21	2.66	7 (41%)
5	NAG	b	2	5	14,14,15	0.56	0	17,19,21	2.13	4 (23%)
5	NAG	e	1	1,5	14,14,15	0.72	1 (7%)	17,19,21	1.72	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Q	407	1	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	0/6/23/26	0/1/1/1
7	NAG	F	201	-	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
7	NAG	U	405	-	-	2/6/23/26	0/1/1/1
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
5	NAG	d	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
6	NAG	f	1	1,6	-	2/6/23/26	0/1/1/1
7	NAG	A	409	1	-	4/6/23/26	0/1/1/1
6	NAG	f	2	6	-	3/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
7	NAG	M	405	1	-	3/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	W	1	1,5	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	3/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
7	NAG	I	405	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
7	NAG	V	201	2	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	NAG	e	1	1,5	-	0/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	405	NAG	C1-C2	4.72	1.58	1.52
6	f	1	NAG	C1-C2	3.78	1.57	1.52
7	M	405	NAG	C1-C2	3.20	1.56	1.52
7	Q	407	NAG	C4-C5	3.16	1.59	1.53
7	V	201	NAG	C1-C2	2.91	1.56	1.52

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	1	NAG	C1-O5-C5	12.26	128.61	112.19
5	c	2	NAG	C1-O5-C5	9.08	124.36	112.19
6	Z	1	NAG	C1-O5-C5	8.18	123.15	112.19
7	I	405	NAG	O5-C1-C2	-8.15	98.68	111.29
7	A	409	NAG	C1-O5-C5	7.94	122.83	112.19

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	NAG	C1-C2-N2-C7
7	Q	407	NAG	C1-C2-N2-C7
6	Z	2	NAG	O5-C5-C6-O6
7	U	405	NAG	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	e	2	NAG	2	0
7	U	405	NAG	5	0
5	g	2	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	f	1	NAG	3	0
6	f	2	NAG	4	0
6	Z	1	NAG	1	0
5	c	1	NAG	1	0
7	I	405	NAG	2	0
5	b	2	NAG	1	0

5.5 Carbohydrates [i](#)

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	W	1	1,5	14,14,15	0.70	0	17,19,21	1.67	4 (23%)
5	NAG	W	2	5	14,14,15	0.69	0	17,19,21	2.61	7 (41%)
5	BMA	W	3	5	11,11,12	1.10	0	15,15,17	3.14	8 (53%)
5	MAN	W	4	5	11,11,12	0.76	0	15,15,17	2.32	3 (20%)
6	NAG	Z	1	1,6	14,14,15	0.91	1 (7%)	17,19,21	2.70	6 (35%)
6	NAG	Z	2	6	14,14,15	0.76	0	17,19,21	1.73	3 (17%)
6	NAG	a	1	1,6	14,14,15	1.02	1 (7%)	17,19,21	2.31	7 (41%)
6	NAG	a	2	6	14,14,15	0.86	1 (7%)	17,19,21	2.24	7 (41%)
5	NAG	b	1	1,5	14,14,15	0.73	0	17,19,21	1.77	4 (23%)
5	NAG	b	2	5	14,14,15	0.56	0	17,19,21	2.13	4 (23%)
5	BMA	b	3	5	11,11,12	0.99	0	15,15,17	2.68	5 (33%)
5	MAN	b	4	5	11,11,12	0.81	0	15,15,17	2.43	6 (40%)
5	NAG	c	1	1,5	14,14,15	0.80	0	17,19,21	3.90	9 (52%)
5	NAG	c	2	5	14,14,15	0.83	1 (7%)	17,19,21	3.80	10 (58%)
5	BMA	c	3	5	11,11,12	0.98	0	15,15,17	3.64	8 (53%)
5	MAN	c	4	5	11,11,12	1.19	2 (18%)	15,15,17	2.68	4 (26%)
5	NAG	d	1	1,5	14,14,15	0.54	0	17,19,21	2.18	4 (23%)
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	2.57	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	d	3	5	11,11,12	0.54	0	15,15,17	2.68	6 (40%)
5	MAN	d	4	5	11,11,12	0.74	0	15,15,17	1.72	3 (20%)
5	NAG	e	1	1,5	14,14,15	0.72	1 (7%)	17,19,21	1.72	5 (29%)
5	NAG	e	2	5	14,14,15	0.56	0	17,19,21	2.44	7 (41%)
5	BMA	e	3	5	11,11,12	1.16	1 (9%)	15,15,17	2.58	5 (33%)
5	MAN	e	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.96	5 (33%)
6	NAG	f	1	1,6	14,14,15	1.15	1 (7%)	17,19,21	2.95	7 (41%)
6	NAG	f	2	6	14,14,15	0.86	0	17,19,21	1.79	5 (29%)
5	NAG	g	1	1,5	14,14,15	0.69	0	17,19,21	1.49	3 (17%)
5	NAG	g	2	5	14,14,15	0.79	0	17,19,21	3.26	10 (58%)
5	BMA	g	3	5	11,11,12	1.21	1 (9%)	15,15,17	2.97	5 (33%)
5	MAN	g	4	5	11,11,12	0.71	0	15,15,17	2.02	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	3/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
5	MAN	b	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	d	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1
5	MAN	d	4	5	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	e	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	BMA	e	3	5	-	2/2/19/22	0/1/1/1
5	MAN	e	4	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	f	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	3/6/23/26	0/1/1/1
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
5	MAN	g	4	5	1/1/4/5	2/2/19/22	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	1	NAG	C1-C2	3.78	1.57	1.52
6	a	2	NAG	C1-C2	2.55	1.55	1.52
5	e	3	BMA	C2-C3	2.49	1.56	1.52
5	c	2	NAG	C3-C2	2.40	1.57	1.52
6	Z	1	NAG	C1-C2	2.38	1.55	1.52

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	1	NAG	C1-O5-C5	12.26	128.61	112.19
5	c	3	BMA	C1-O5-C5	9.97	125.55	112.19
5	c	2	NAG	C1-O5-C5	9.08	124.36	112.19
5	c	4	MAN	C1-O5-C5	-8.41	100.91	112.19
6	Z	1	NAG	C1-O5-C5	8.18	123.15	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	W	4	MAN	C1
5	b	4	MAN	C1
5	c	4	MAN	C1
5	d	4	MAN	C1
5	e	4	MAN	C1

5 of 48 torsion outliers are listed below:

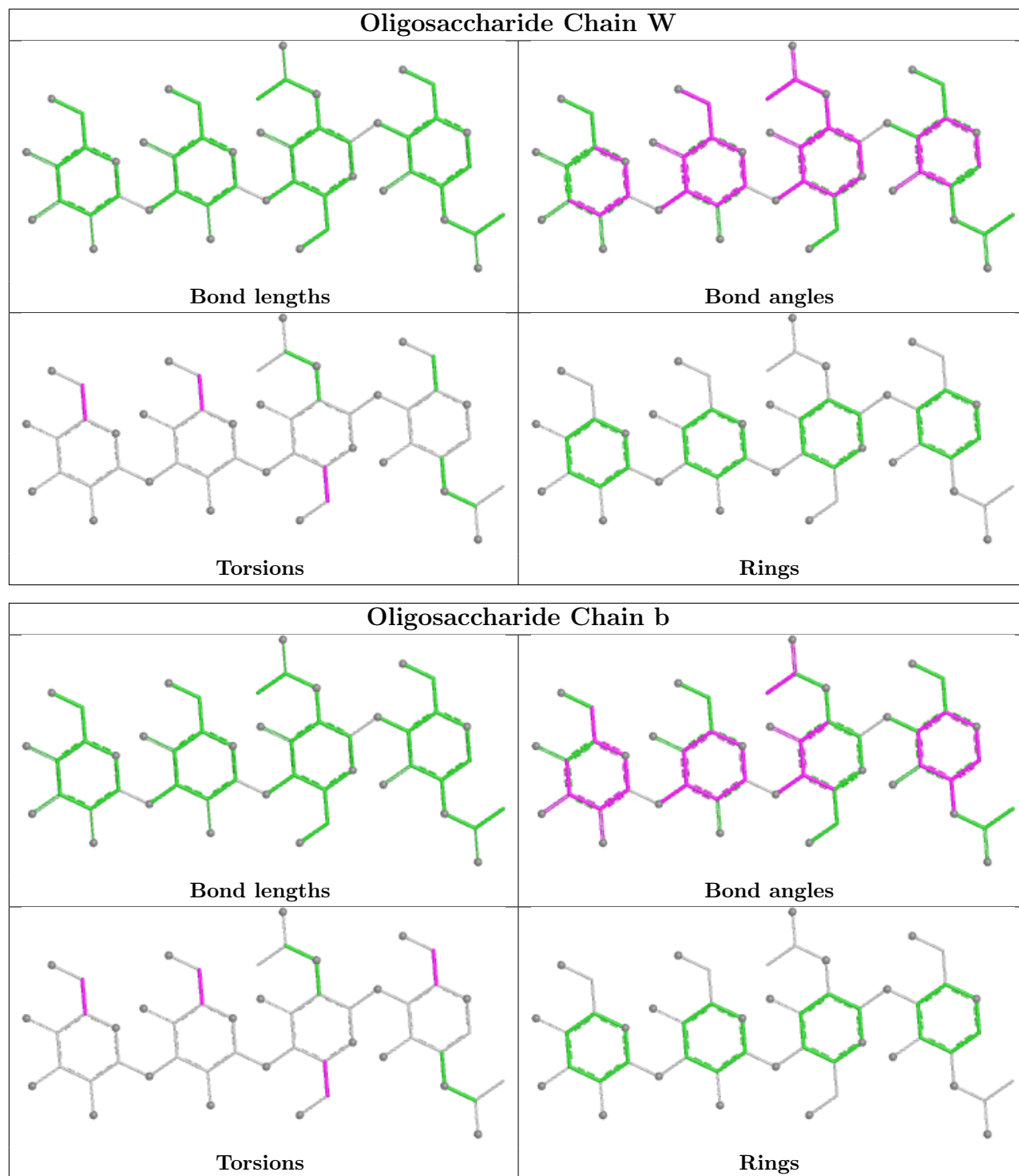
Mol	Chain	Res	Type	Atoms
5	W	4	MAN	C4-C5-C6-O6
5	g	4	MAN	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	g	3	BMA	C4-C5-C6-O6

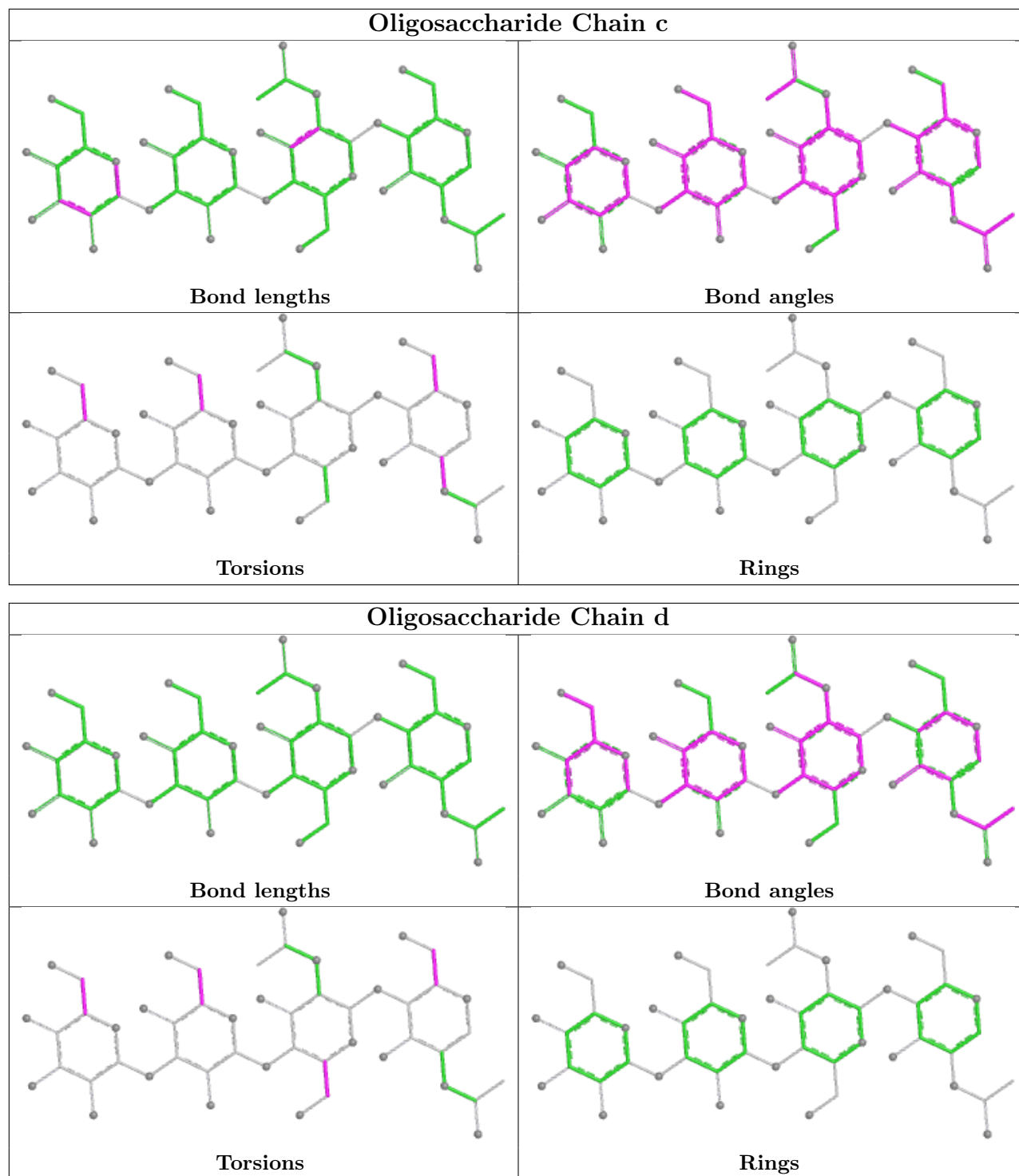
There are no ring outliers.

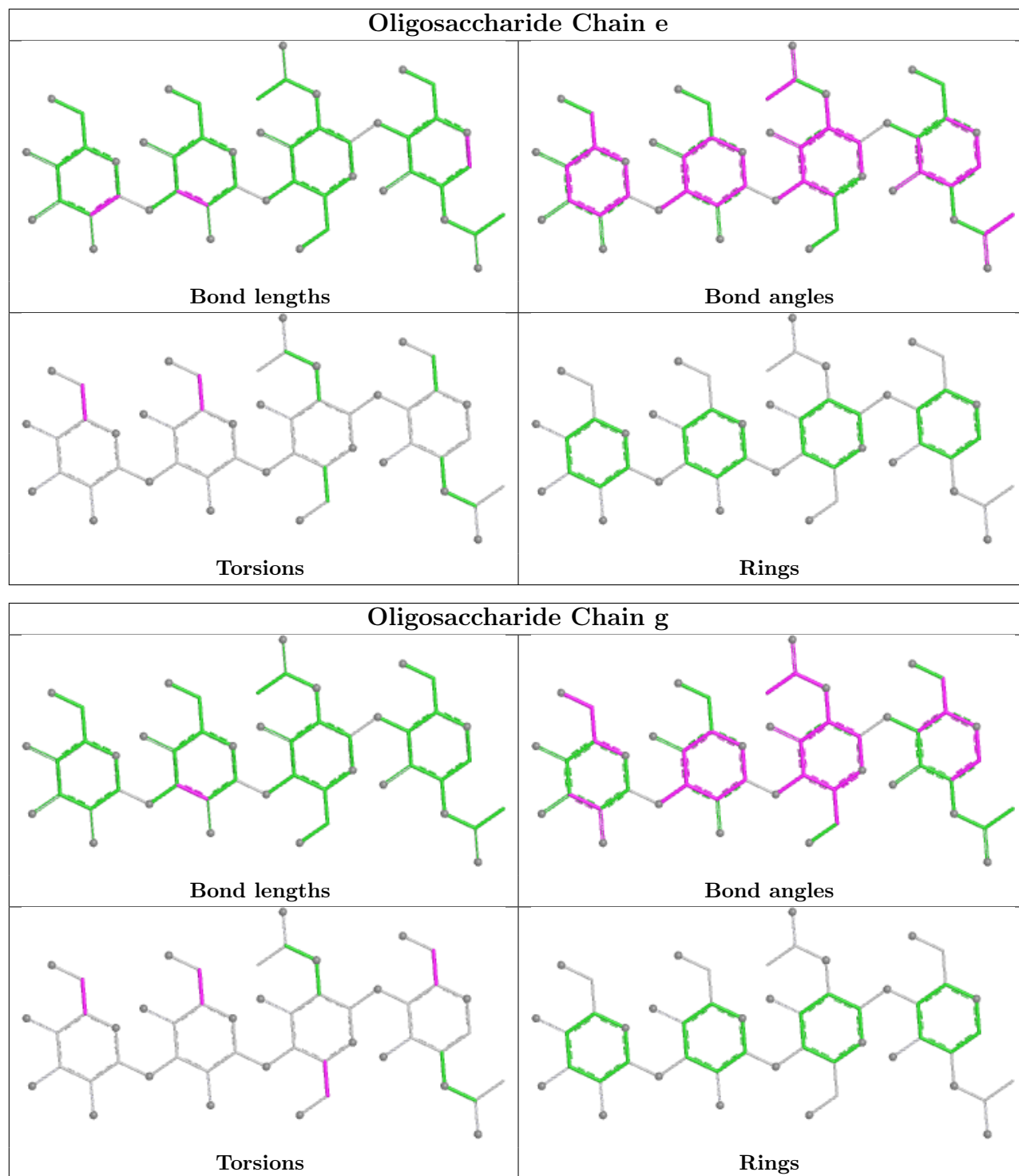
11 monomers are involved in 15 short contacts:

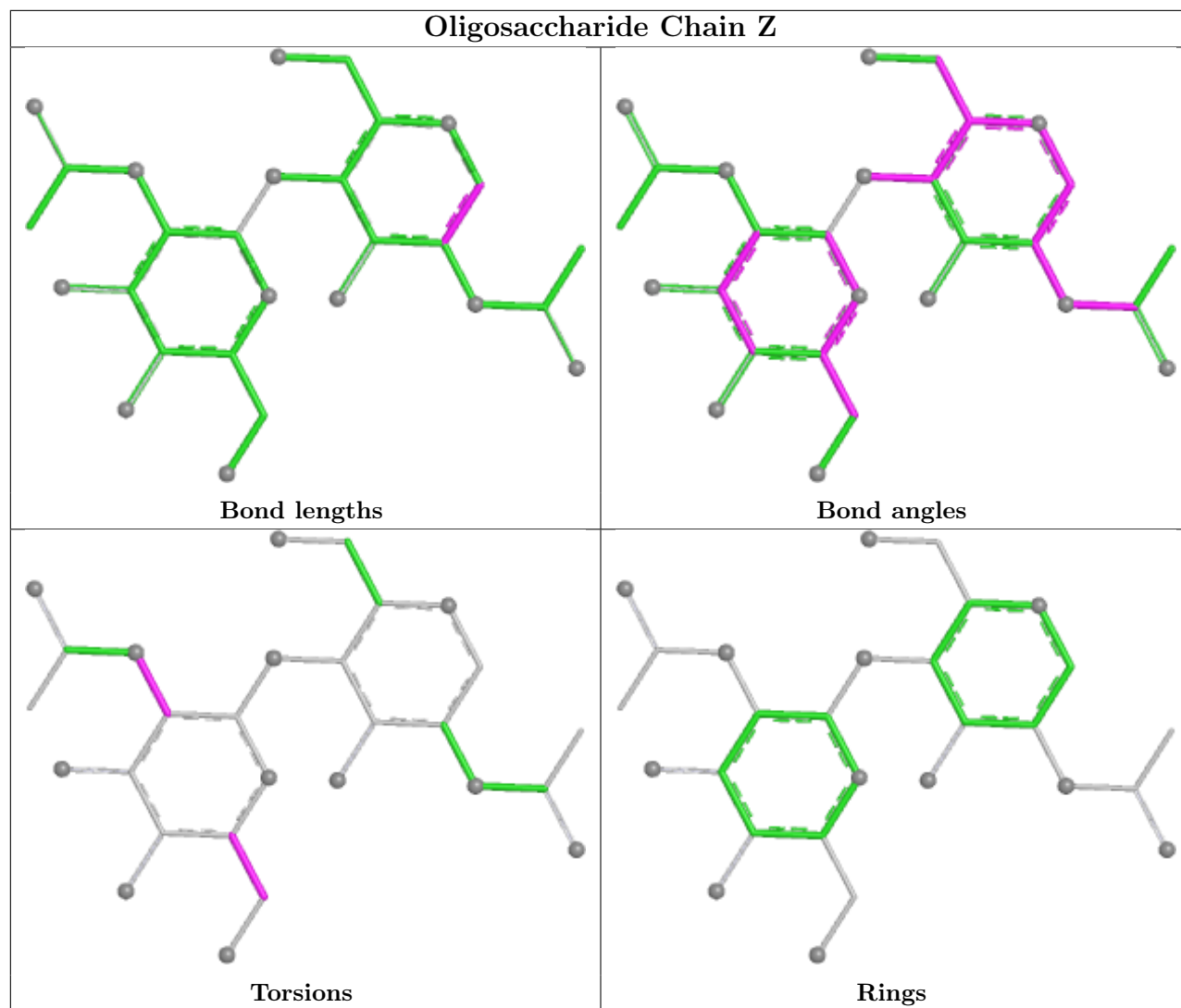
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	b	4	MAN	1	0
5	e	2	NAG	2	0
5	b	3	BMA	1	0
5	g	2	NAG	1	0
6	f	1	NAG	3	0
6	f	2	NAG	4	0
6	Z	1	NAG	1	0
5	c	1	NAG	1	0
5	g	3	BMA	1	0
5	g	4	MAN	1	0
5	b	2	NAG	1	0

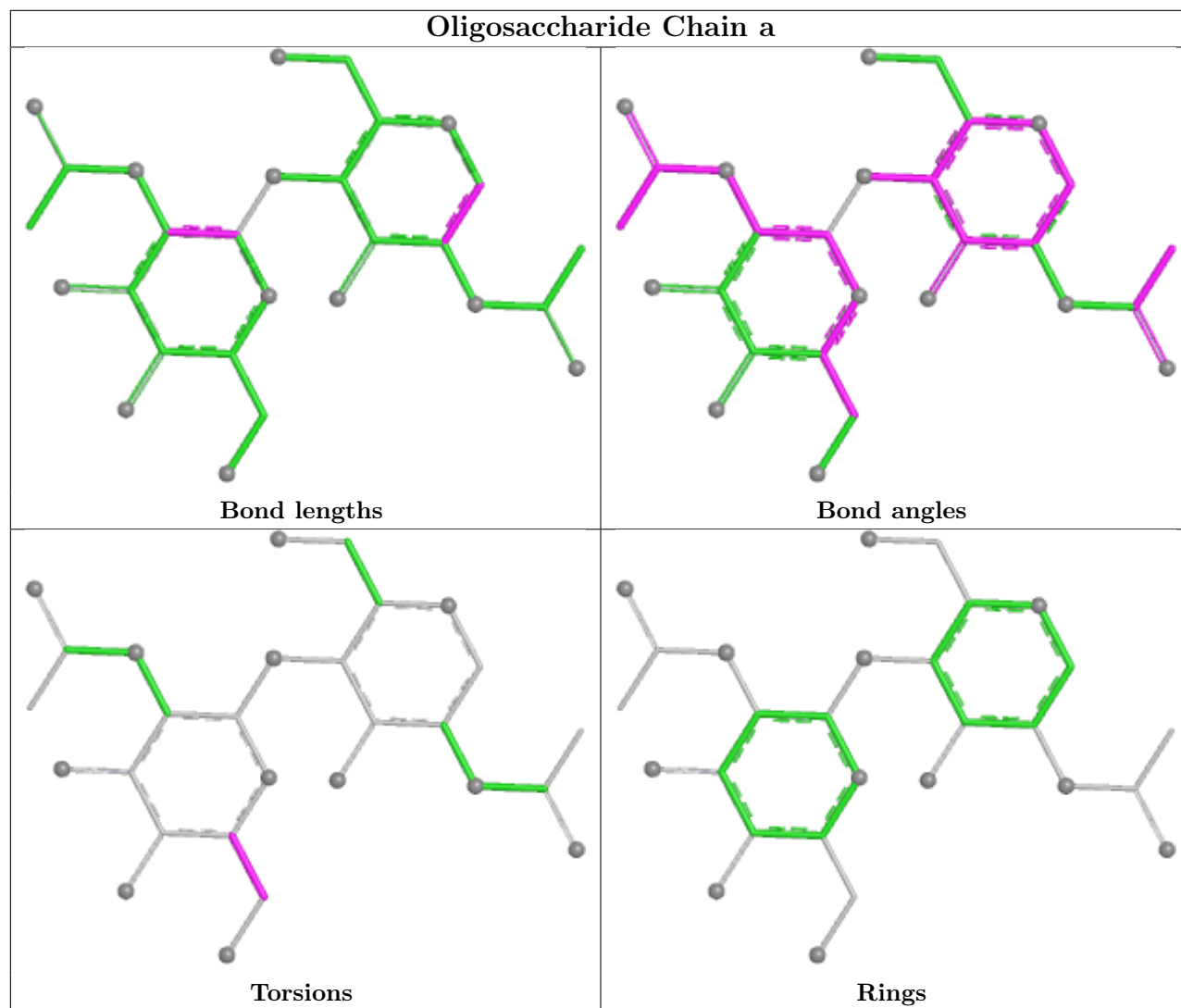
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

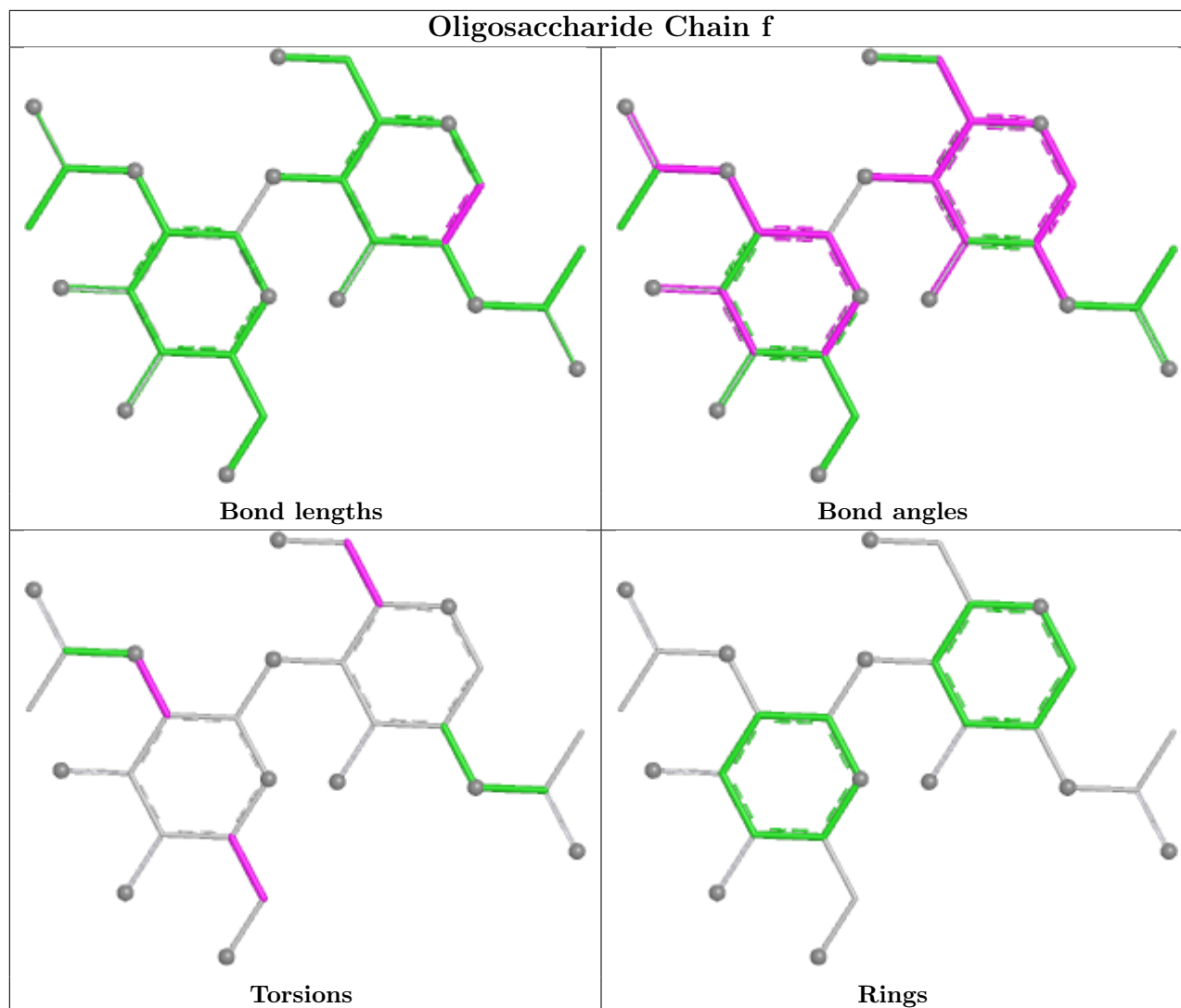












5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	NAG	U	405	-	14,14,15	1.34	2 (14%)	17,19,21	2.96	9 (52%)
7	NAG	Q	407	1	14,14,15	1.43	3 (21%)	17,19,21	3.39	9 (52%)
7	NAG	I	405	1	14,14,15	1.68	2 (14%)	17,19,21	3.24	11 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	409	1	14,14,15	1.06	1 (7%)	17,19,21	3.33	8 (47%)
7	NAG	V	201	2	14,14,15	1.05	1 (7%)	17,19,21	2.66	7 (41%)
7	NAG	M	405	1	14,14,15	1.09	1 (7%)	17,19,21	1.34	3 (17%)
7	NAG	F	201	-	14,14,15	0.99	0	17,19,21	2.24	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	U	405	-	-	2/6/23/26	0/1/1/1
7	NAG	Q	407	1	-	4/6/23/26	0/1/1/1
7	NAG	I	405	1	-	0/6/23/26	0/1/1/1
7	NAG	A	409	1	-	4/6/23/26	0/1/1/1
7	NAG	V	201	2	-	2/6/23/26	0/1/1/1
7	NAG	M	405	1	-	3/6/23/26	0/1/1/1
7	NAG	F	201	-	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	405	NAG	C1-C2	4.72	1.58	1.52
7	M	405	NAG	C1-C2	3.20	1.56	1.52
7	Q	407	NAG	C4-C5	3.16	1.59	1.53
7	V	201	NAG	C1-C2	2.91	1.56	1.52
7	U	405	NAG	C3-C2	2.89	1.58	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	405	NAG	O5-C1-C2	-8.15	98.68	111.29
7	A	409	NAG	C1-O5-C5	7.94	122.83	112.19
7	Q	407	NAG	C1-O5-C5	6.98	121.54	112.19
7	V	201	NAG	C1-O5-C5	6.93	121.47	112.19
7	Q	407	NAG	O4-C4-C5	5.67	123.28	109.32

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	NAG	C1-C2-N2-C7
7	Q	407	NAG	C1-C2-N2-C7
7	U	405	NAG	O5-C5-C6-O6
7	A	409	NAG	O5-C5-C6-O6
7	V	201	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	405	NAG	5	0
7	I	405	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/321 (99%)	-1.22	0 100 100	68, 103, 128, 172	0
1	E	320/321 (99%)	-1.20	1 (0%) 90 76	57, 99, 124, 184	0
1	I	317/321 (98%)	-1.23	0 100 100	57, 93, 117, 143	0
1	M	320/321 (99%)	-1.21	0 100 100	60, 94, 118, 199	0
1	Q	320/321 (99%)	-1.18	0 100 100	57, 99, 129, 188	0
1	U	320/321 (99%)	-1.19	0 100 100	67, 103, 132, 177	0
2	B	165/175 (94%)	-1.18	0 100 100	58, 94, 129, 183	0
2	F	163/175 (93%)	-1.08	0 100 100	66, 104, 139, 175	0
2	J	164/175 (93%)	-1.02	0 100 100	63, 104, 138, 178	0
2	N	163/175 (93%)	-1.04	0 100 100	64, 102, 135, 163	0
2	R	166/175 (94%)	-1.10	0 100 100	64, 103, 141, 185	0
2	V	164/175 (93%)	-1.21	0 100 100	59, 94, 129, 171	0
3	C	219/226 (96%)	-1.18	0 100 100	70, 96, 142, 202	0
3	G	219/226 (96%)	-1.14	0 100 100	77, 117, 170, 219	0
3	K	219/226 (96%)	-0.80	0 100 100	100, 175, 253, 286	0
3	O	219/226 (96%)	-0.65	3 (1%) 73 48	111, 189, 304, 357	0
3	S	219/226 (96%)	-1.08	1 (0%) 87 68	83, 117, 169, 217	0
3	Y	219/226 (96%)	-1.18	0 100 100	70, 95, 145, 206	0
4	D	213/215 (99%)	-1.13	0 100 100	69, 96, 127, 156	0
4	H	213/215 (99%)	-1.06	0 100 100	75, 115, 164, 197	0
4	L	213/215 (99%)	-0.85	1 (0%) 87 68	99, 186, 239, 267	0
4	P	213/215 (99%)	-0.73	0 100 100	96, 205, 273, 317	0
4	T	213/215 (99%)	-1.06	0 100 100	76, 115, 170, 216	0
4	X	213/215 (99%)	-1.14	0 100 100	69, 95, 126, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5494/5622 (97%)	-1.09	6 (0%) 92 86	57, 105, 215, 357	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	164	THR	3.5
4	L	135	CYS	2.7
3	O	192	SER	2.6
1	E	12	THR	2.4
3	O	194	VAL	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	W	1	14/15	-	-	105,108,112,113	0
5	NAG	W	2	14/15	-	-	108,122,129,133	0
7	NAG	F	201	14/15	0.92	0.06	155,185,196,198	0
7	NAG	V	201	14/15	0.97	0.06	103,112,121,121	0
6	NAG	a	1	14/15	-	-	179,195,202,203	0
6	NAG	a	2	14/15	-	-	151,173,185,190	0
7	NAG	I	405	14/15	0.98	0.05	106,126,133,137	0
5	NAG	b	1	14/15	-	-	120,124,127,128	0
5	NAG	b	2	14/15	-	-	102,125,137,141	0
7	NAG	M	405	14/15	0.98	0.06	101,119,136,138	0
6	NAG	Z	2	14/15	0.98	0.07	147,155,164,165	0
5	NAG	c	1	14/15	-	-	85,91,92,92	0
5	NAG	c	2	14/15	-	-	101,107,116,121	0
7	NAG	A	409	14/15	0.99	0.03	89,104,118,124	0
5	NAG	d	1	14/15	-	-	90,94,96,97	0
5	NAG	d	2	14/15	-	-	94,104,111,111	0
7	NAG	U	405	14/15	0.99	0.03	84,97,121,129	0
5	NAG	e	1	14/15	-	-	96,104,115,116	0
5	NAG	e	2	14/15	-	-	107,116,134,136	0
6	NAG	f	1	14/15	-	-	112,128,138,152	0
6	NAG	f	2	14/15	-	-	152,179,197,197	0
7	NAG	Q	407	14/15	0.99	0.03	85,101,107,107	0

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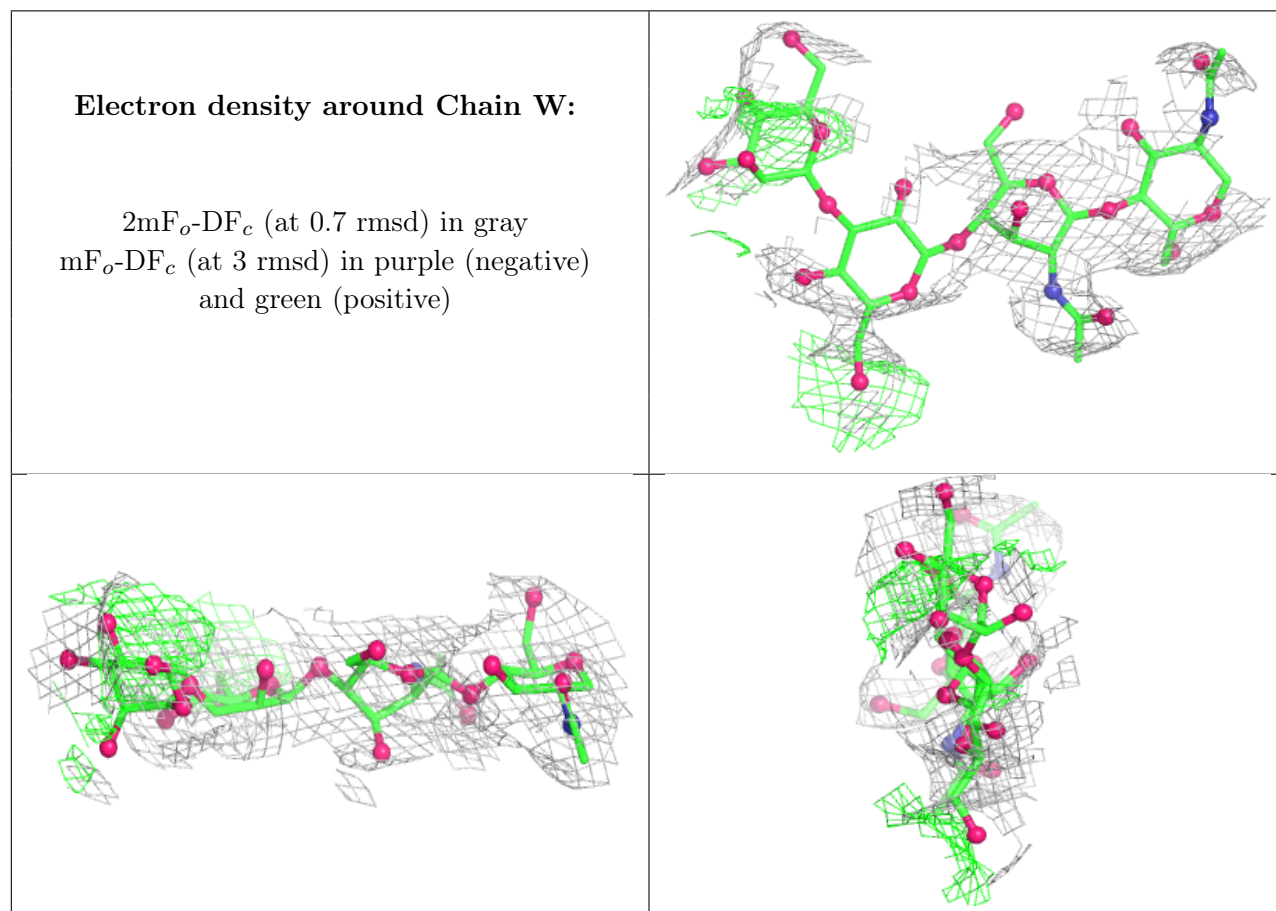
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	g	1	14/15	-	-	101,108,117,119	0
5	NAG	g	2	14/15	-	-	102,121,142,146	0
6	NAG	Z	1	14/15	0.99	0.04	130,133,144,145	0

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

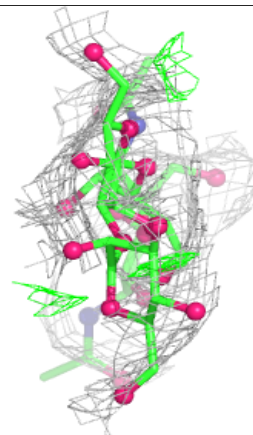
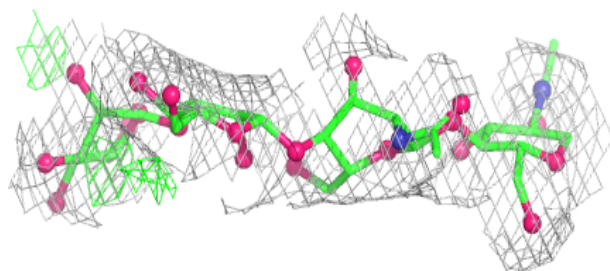
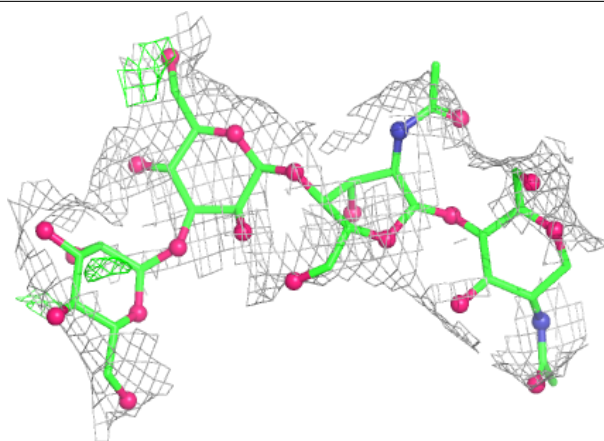
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	W	1	14/15	-	-	105,108,112,113	0
5	NAG	W	2	14/15	-	-	108,122,129,133	0
5	BMA	W	3	11/12	-	-	109,123,131,147	0
5	MAN	W	4	11/12	-	-	147,149,156,160	0
5	NAG	b	1	14/15	-	-	120,124,127,128	0
5	NAG	b	2	14/15	-	-	102,125,137,141	0
5	BMA	b	3	11/12	-	-	114,124,135,146	0
5	MAN	b	4	11/12	-	-	135,149,150,150	0
5	NAG	c	1	14/15	-	-	85,91,92,92	0
5	NAG	c	2	14/15	-	-	101,107,116,121	0
5	BMA	c	3	11/12	-	-	104,110,118,121	0
5	MAN	c	4	11/12	-	-	134,140,148,169	0
5	NAG	d	1	14/15	-	-	90,94,96,97	0
5	NAG	d	2	14/15	-	-	94,104,111,111	0
5	BMA	d	3	11/12	-	-	106,111,126,130	0
5	MAN	d	4	11/12	-	-	141,147,157,173	0
5	NAG	e	1	14/15	-	-	96,104,115,116	0
5	NAG	e	2	14/15	-	-	107,116,134,136	0
5	BMA	e	3	11/12	-	-	107,121,124,132	0
5	MAN	e	4	11/12	-	-	129,145,149,150	0
5	NAG	g	1	14/15	-	-	101,108,117,119	0
5	NAG	g	2	14/15	-	-	102,121,142,146	0
5	BMA	g	3	11/12	-	-	116,129,135,137	0
5	MAN	g	4	11/12	-	-	125,138,145,146	0
6	NAG	Z	2	14/15	0.98	0.07	147,155,164,165	0
6	NAG	Z	1	14/15	0.99	0.04	130,133,144,145	0
6	NAG	a	1	14/15	-	-	179,195,202,203	0
6	NAG	a	2	14/15	-	-	151,173,185,190	0
6	NAG	f	1	14/15	-	-	112,128,138,152	0
6	NAG	f	2	14/15	-	-	152,179,197,197	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

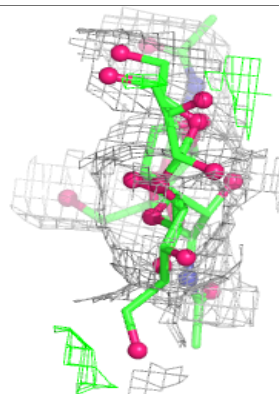
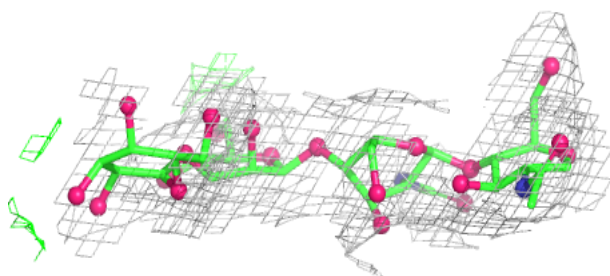
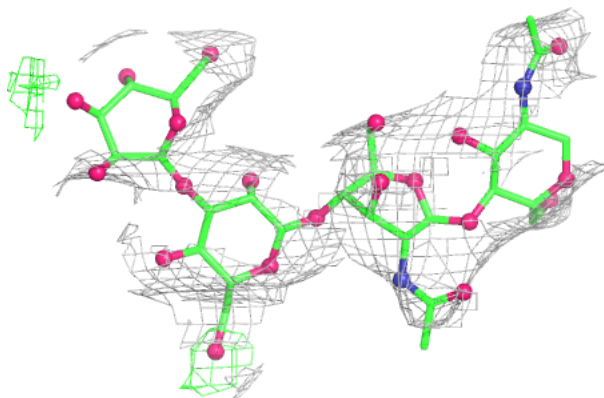


Electron density around Chain b:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

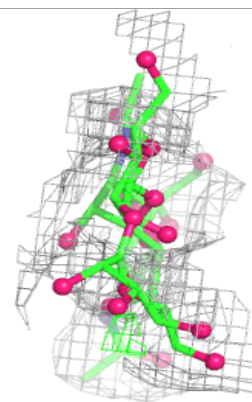
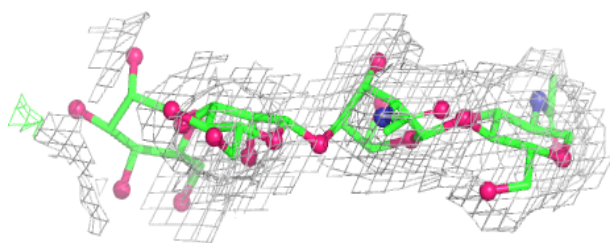
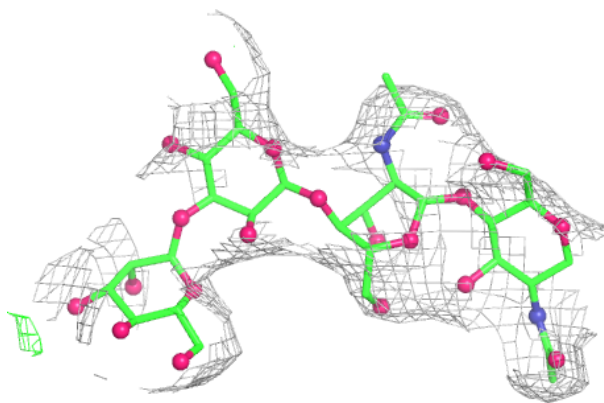
**Electron density around Chain c:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

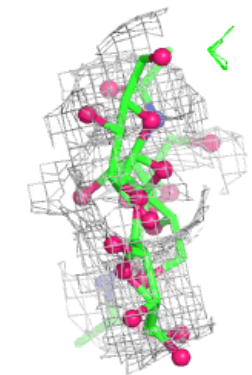
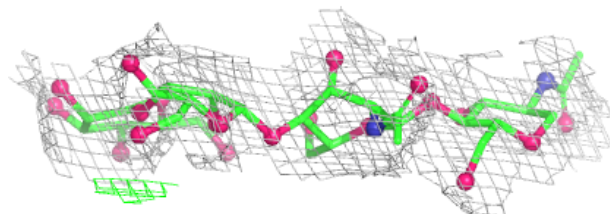
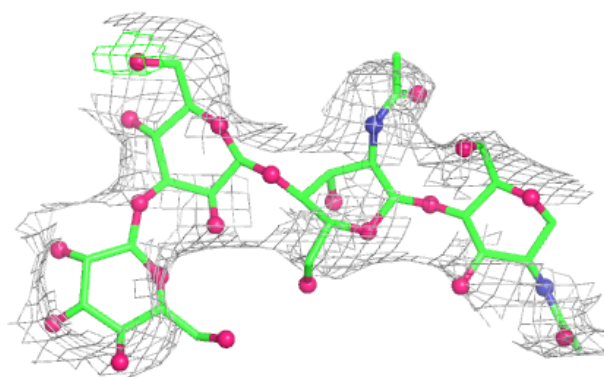


Electron density around Chain d:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

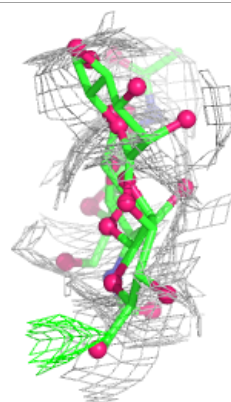
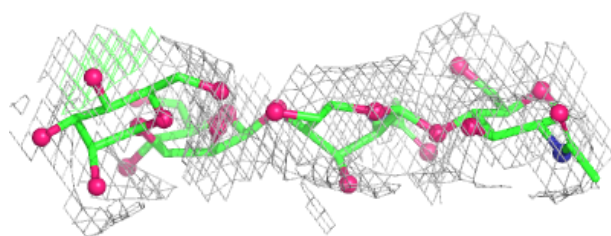
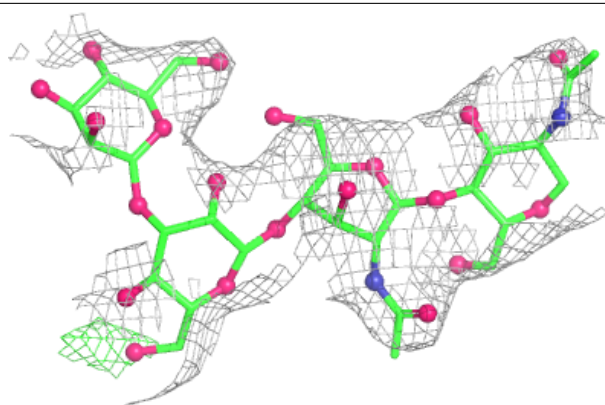
**Electron density around Chain e:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

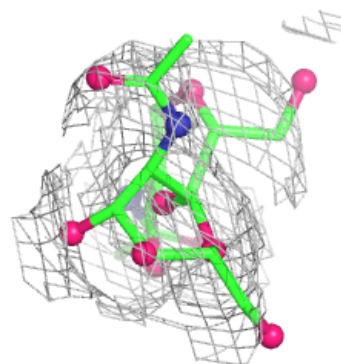
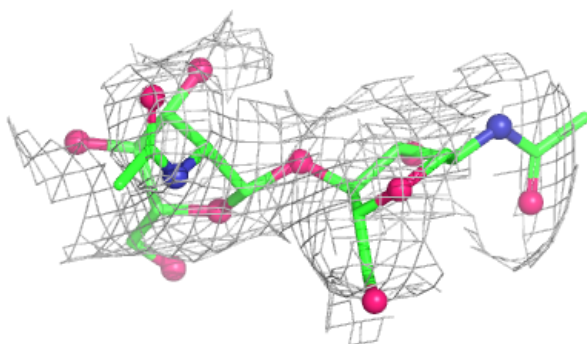
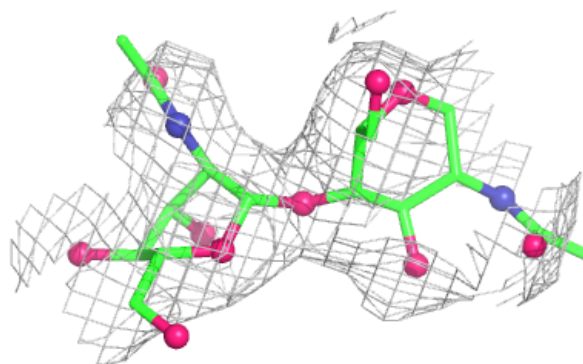


Electron density around Chain g:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

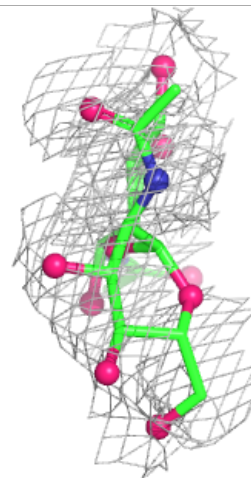
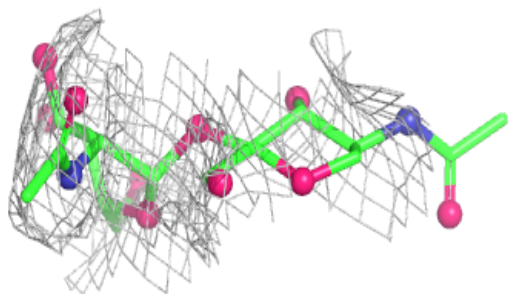
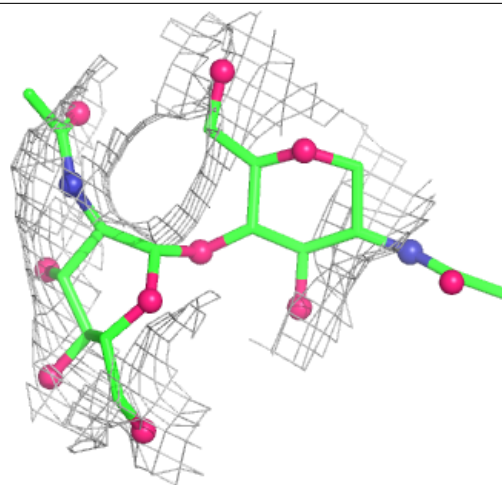
**Electron density around Chain Z:**

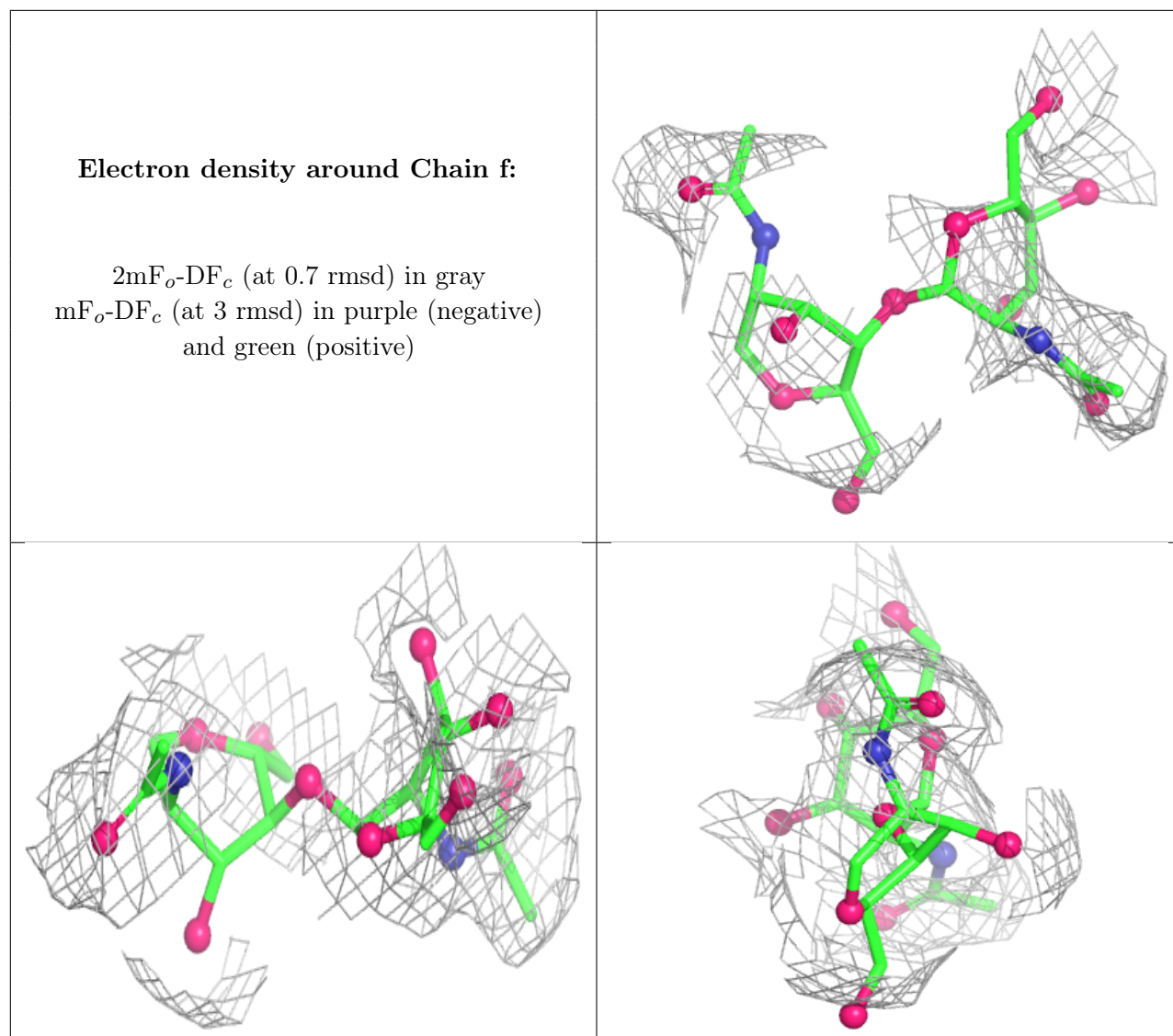
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	F	201	14/15	0.92	0.06	155,185,196,198	0
7	NAG	V	201	14/15	0.97	0.06	103,112,121,121	0
7	NAG	M	405	14/15	0.98	0.06	101,119,136,138	0
7	NAG	I	405	14/15	0.98	0.05	106,126,133,137	0
7	NAG	A	409	14/15	0.99	0.03	89,104,118,124	0
7	NAG	Q	407	14/15	0.99	0.03	85,101,107,107	0
7	NAG	U	405	14/15	0.99	0.03	84,97,121,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.